

Wang, S. X., Wang, L. M., & Ewing, R. C. (1999). Electron irradiation of zeolites. In Zinkle, S. J., Lucas, G. E., Ewing, R. C., & Williams, J. S. (Eds.), *Microstructural Processes in Irradiated Materials*. Symposium Proceedings of the Materials Research Society. 540, 361-366.

## **SPENT NUCLEAR FUEL**

### **Engineering Science**

**Project: 60144**

*Title:* Flow Visualization of Forced and Natural Convection in Internal Cavities

*PI:* Dr. John C. Crepeau

*Institution:* University of Idaho

*Publication Type:* Journal

Condie, K. G., Stoots, C. M., McEligot, D. M., Becker, S., & Durst, F. (1998). Measurements of induced boundary layer transition in the new INEEL Matched-Index-of-Refractive flow system. American Physical Society Fluid Dynamics Meeting. Bulletin APS. 43, 2092.

Nishimura, M., Fujii, S., Shehata, A. M., Kunugi, T., & McEligot, D. M. (1997). Prediction of forced gas flows in circular tubes at high heat fluxes. NuReTH-8, Kyoto.

Shehata, A. M. & McEligot, D. M. (1998). Mean structure in the viscous layer of strongly-heated internal gas flows. International Journal of Heat Mass Transfer. 41, 4297-4313.

*Publication Type:* Presentation

Crepeau, J. C. (2000, Sep. 13). Drying of spent nuclear fuel. Presentation for the Mechanical Engineering Department of the University of Idaho Extension, Idaho Falls, ID.

Ezato, K., Shehata, A. M., Kunugi, T., & McEligot, D. M. (1997). Numerical predictions of transitional features of turbulent forced gas flows in circular tubes with strong heating. ASME Fluids Engineering Conference. Vancouver, British Columbia, Canada.

McEligot, D. M. (1997). Maximum allowable heat flux for a submerged tube bundle. Engineering Conference on Convective Flow and Pool Boiling. Irsee, Germany.

McEligot, D. M., Shehata, A. M., & Kunugi, T. (1998). Prediction of strongly-heated gas flows. Invited presentation at the Engineering Foundation Conference on Turbulent Heat Transfer II, I. 33-47. Manchester, U. K.

*Publication Type: Proceeding*

Crepeau, J. C., et. al. (1998, Sept.). Fluid mechanic studies relating to drying and passivation in an idealized SNF cannister. ANS 3rd Topical Meeting on Spent Nuclear Fuel and Fissile Material Management. Charleston, SC.

McCreery, G. E. & Martineau, R. M. (1998, Nov.). An experimental investigation of steam injection in fractured porous media. ASME International Mechanical Engineering Congress. Anaheim, CA.

McCreery, G. E., et. al. (1999, Sept. 6-9). Flow visualization and velocity measurements in a model fuel storage canister. ANS Global '99 International Conference on Future Nuclear Systems. Jackson, WY.

McCreery, G. E., Kullberg, C. M., Schultz, R. R., Yonomoto, T., & Anoda, Y. (1997). Heat transfer modeling of the LSTF Passive Residual Heat Removal System. ASME Nuclear Engineering Division, ASME Symposium of the 1997 International Mechanical Engineering Congress. Dallas, TX. 97-106.

**Geochemistry****Project: 59849**

*Title:* Radionuclide Immobilization in the Phases Formed by Corrosion of Spent Nuclear Fuel: The Long-Term Assessment

*PI:* Dr. Rodney C. Ewing *Institution:* University of Michigan

*Publication Type:* Paper

Jensen, K. A. & Ewing, R. C. (2000). The Okelobondo natural fission reactor, southeast Gabon: Geology, mineralogy, and retardation of nuclear-reaction products. Geological Society of America Bulletin. 113(1), 32-62.

**Project: 73691 (Renewal of Project No. 59960)**

*Title:* Renewal of Direct Investigations of the Immobilization of Radionuclides in the Alteration Products of Spent Nuclear Fuel

*PI:* Dr. Peter C. Burns *Institution:* University of Notre Dame

*Publication Type:* Journal

Burns, P. C. & Finch, R.J. (1999, Sep.). Wyartite: Crystallographic evidence for the first pentavalent-uranium mineral. Am. Mineral. 84(9), 1456-1460.

Burns, P. C. & Hill, F. C. (2000, Feb.). A new uranyl sheet in K-5[(UO<sub>2</sub>)(10)O-8(OH)(9)](H<sub>2</sub>O): New insight into sheet anion-topologies. Can. Mineral. 38, 163-173, Part 1.

Burns, P. C. & Hill, F. C. (2000, Feb.). Implications of the synthesis and structure of the Sr analogue of curite. Can. Mineral. 38, 175-181, Part 1.

Burns, P. C. (1998). The structure of boltwoodite and implications of solid-solution towards sodium boltwoodite. *Canadian Mineralogist*. 36, 1069-1075.

Burns, P. C. (1998). The structure of compreignacite,  $K_2[(UO_2)_3O_2(OH)_3]_2(H_2O)_7$ . *Canadian Mineralogist*. 36, 1061-1067.

Burns, P. C. (1999). Cs boltwoodite obtained by ion exchange from single crystals: Implications for radionuclide release in a nuclear repository. *J. Nucl. Mater.* 265, 218-223.

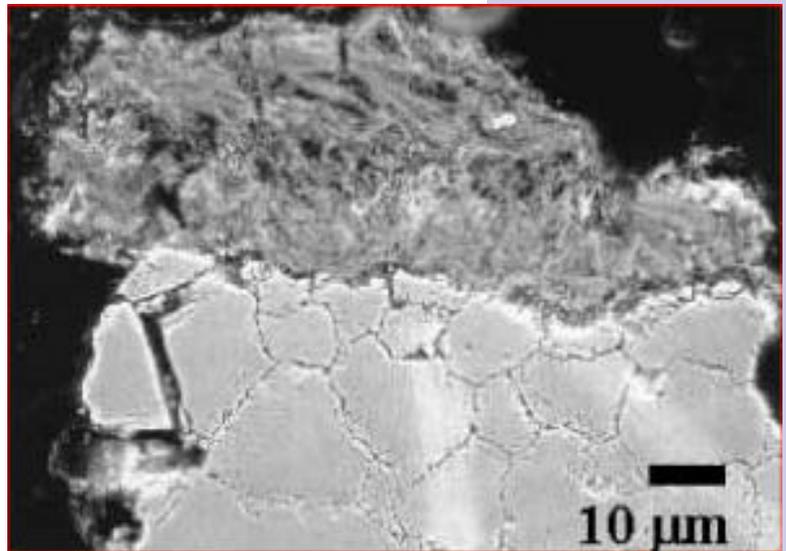
Burns, P. C., Olson, R. A., Finch, R. J., Hanchar, J. M., & Thibault, Y. (1999).  $KNa_3(UO_2)_2(Si_4O_{10})_2(H_2O)_4$ , a new compound formed during vapor hydration of an actinide-bearing borosilicate waste glass. *J. Nucl. Mater.* 278(2-3), 290-300.

Burns, P.C. (2000, May-Jun.). A new uranyl phosphate chain in the structure of parsonsite. *Am. Mineral.* 85(5-6), 801-805.

Chen, F. R., Burns, P. C., & Ewing, R. C. (2000, Apr.). Near-field behavior of Tc-99 during the oxidative alteration of spent nuclear fuel. *J. Nucl. Mater.* 278(2-3), 225-232.

Chen, F., Burns, P. C., & Ewing, R. C. (1999, Oct.). Se-79: Geochemical and crystallo-chemical retardation mechanisms. *J. Nucl. Mater.* 275(1), 81-94.

Hill, F.C. & Burns, P.C. (1999, Oct.). The structure of a synthetic Cs uranyl oxide hydrate and its relationship to compreignacite. *Can. Mineral.* 37, 1283-1288, Part 5.



Laboratory Studies: Argonne National Labs  
High Drip Rate Tests:

Alteration Phases:

Boltwoodite:  $(K,Na)[(UO_2)(SiO_3OH)](H_2O)_{1.5}$

Uranophane:  $Ca[(UO_2)(SiO_3OH)]_2(H_2O)_5$

[see Project #73691, renewal of #59960]



The mineral uraninite,  $UO_2$ , is an excellent natural analogue for  $UO_2$  (LWR) spent fuel. This photograph shows a specimen of uraninite (black) that has been oxidized under conditions broadly similar to those that will be present in the proposed repository at Yucca Mountain. The uranyl phases that have formed due to the alteration (oxidation) are clearly visible as yellow and orange crystals. We obtain many of the crystals used in our studies from similar natural occurrences. These minerals are typically identical to the phases that form when spent fuel is corroded during laboratory tests at ANL. [see Project #73691, renewal of #59960]

*Publication Type: Paper*

Burns, P. C. (1999, in press). The crystal chemistry of uranium. Mineralogical Society of America Reviews in Mineralogy.

*Publication Type: Presentation*

Burns, P. C. & Finch, R. J. (1999). The structure of wyartite: Crystallographic evidence for the first pentavalent-uranium mineral. GAC-MAC. Sudbury, Ontario, Canada.

Burns, P. C. (1998): Topological aspects of uranyl mineral structures. IMA. Toronto, Canada.

Burns, P. C., Finch, R. C. & Wronkiewicz, D. J. (1998). Direct investigations of the immobilization of radionuclides in the alteration products of spent nuclear fuel. DOE Environmental Management Science Program Workshop. Chicago, IL.

Hill, F. C. & Burns, P. C. (1998). Chemical and structural diversity in the uranyl oxide hydrate system. GSA Toronto, Canada.

Hill, F. C. & Burns, P. C. (1998). Investigations of the crystal chemistry of uranyl oxide hydrates. IMA Toronto, Canada.

Hill, F. C. & Burns, P. C. (1999). The importance of uranyl silicates for the disposal of nuclear waste. GAC-MAC. Sudbury, Ontario, Canada.

Kim, C. W. & Wronkiewicz, D. J. (1998). Alteration phases of spent nuclear fuel. Missouri Academy of Sciences, 1998 Annual Meeting.

*Publication Type: Proceeding*

Chen, F., Burns, P.C., & Ewing, R.C. (1998, in press). 79-Se: Geochemical and crystallo-chemical retardation mechanisms. The Scientific Basis for Nuclear Waste Management XX. MRS Proceedings.

**Project: 73751 (Renewal of Project No. 59849)**

*Title:* Corrosion of Spent Nuclear Fuel: The Long Term Assessment

*PI:* Dr. Rodney C. Ewing

*Institution:* University of Michigan

*Publication Type: Journal*

Casas, I., et. al. (1998). The role of pe, pH, and carbonate on the solubility of UO<sub>2</sub> and uraninite under nominally reducing conditions. *Geochimica et Cosmochimica Acta*. 62(13), 2223-2231.

Chen, F. & Ewing, R. C. (1999, in press). Structural contributions to the third-law entropies of uranyl phases. *Geochimica et Cosmochimica Acta*.

Chen, F., Burns, P. C., & Ewing, R. C. (1999). 79-Se: Geochemical and crystallochemical retardation mechanisms. *J. Nucl. Mater.* 275, 81-94.

Chen, F., Burns, P. C., & Ewing, R. C. (1999, in press). Near-field behavior of 99-Tc during the oxidative alteration of spent nuclear fuel. *J. Nucl. Mater.*

Chen, F., Ewing, R. C., & Clark, S. B. (1999). The Gibbs free energies and enthalpies of formation of uranium (VI) phases: An empirical method of prediction. *American Mineralogist.* 84(4), 650-654.

Clark, S. B., Ewing, R. C., & Schaumlöffel, J. C. (1998). A method to predict free energies of formation of mineral phases in the U(VI)-SiO<sub>2</sub>-H<sub>2</sub>O system. *Journal of Alloys and Compounds.* 271, 189-193.

Ewing, R. C. (1999). Less geology in the geological disposal of nuclear waste. *Science.* 286, 415-416.

Ewing, R. C., Tierney, M. S., Konikow, L. F., & Rechar, R. P. (1999). Performance assessments of nuclear waste repositories: A dialogue on their value and limitations. *Risk Analysis.* 19(5), 933-958.

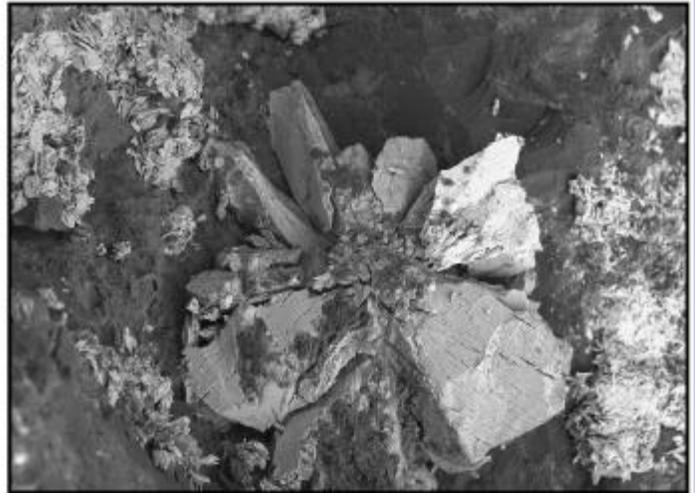
Fayek, M., Burns, P., Guo, Y. -X., & Ewing, R. C. (2000). Micro-structures associated with uraninite alteration. *J. Nucl. Mater.* 277, 204-210.

Finch, R. J., Cooper, M. A., Hawthorne, F. C., & Ewing, R. C. (1999). Refinement of the crystal structure of rutherfordine. *Canadian Mineralogist.* 37, 929-938.

Finch, R. J., Hawthorne, F. C., & Ewing, R. C. (1998). Structural relations among schoepite, metaschoepite, and "dehydrated schoepite." *Canadian Mineralogist.* 36, 831-845.

Jensen, K. A. & Ewing, R. C. (1999, in press). The Okelobondo natural fission reactor, southeast Gabon: Geology, mineralogy, and retardation of nuclear reaction products. *Geological Society of America Bulletin.*

Zhao, D. & Ewing, R. C. (2000, in press). Alteration products of uraninite from the Colorado Plateau. *Radiochimica Acta.*



SEM-image of a sandstone sample from a U-deposit open pit in Oklo-Okélobondo in Gabon of West-Central Africa, coated with aggregates of johanneite, uranyl sulfate hydroxide hydrate, silica, and kaolinite. [see Project #73751, renewal of #59849]

*Publication Type: Presentation*

Ewing, R. C. (1999, Apr. 22). Radiation effects in AB04 orthophosphates and orthosilicates. Invited presentation at the HLW and Pu Immobilization Workshop, CEA. Saclay, France.

Ewing, R. C. (1999, Apr. 5). Performance assessments: The design, selection and importance of nuclear waste forms. Invited presentation at the Chemistry Division Colloquium, Argonne National Laboratory. Argonne, IL.

Ewing, R. C. (1999, Jul. 12). Ageing studies of nuclear waste forms: The evaluation of long-term behaviour. Plenary lecture at the International Conference on Ageing Studies & Lifetime Extension of Materials. St. Catherine's College. Oxford, United Kingdom.

Ewing, R. C. (1999, Jun. 1). The Yucca Mountain Repository: What has changed? Invited presentation at the American Geophysical Union, Spring Meeting. Boston, MA.

Ewing, R. C. (1999, Nov. 13). Mineralogy: Applications to nuclear waste disposal. Plenary presentation at the Twentieth Annual New Mexico Mineral Symposium. New Mexico Institute of Mining and Technology. Socorro, NM.

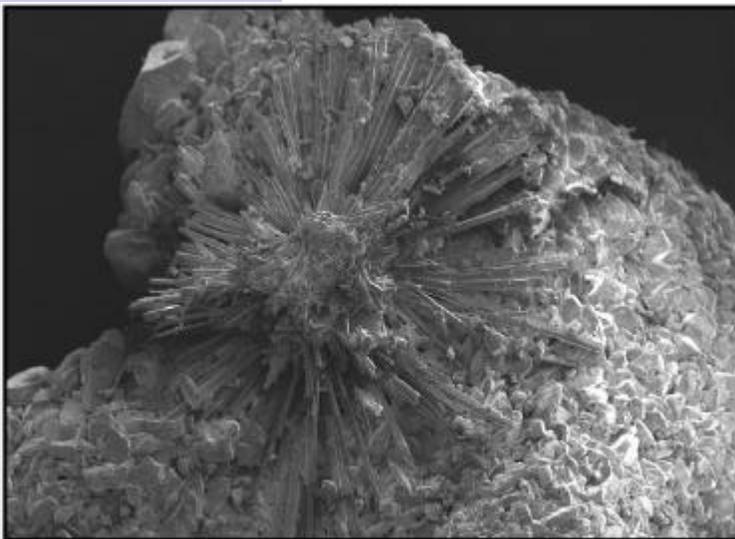
Ewing, R. C. (1999, Oct. 20). Natural systems: Applications to nuclear waste management. Invited presentation at a workshop sponsored by the Russian Academy of Sciences and the U. S. Department of Energy. Moscow, Russia.

Ewing, R. C. (1999, Sep. 10). Radiation effects in zircon. Invited seminar at the Universite Henri Poincare. Nancy, France.

Ewing, R. C. (1999, Sept. 26 - Oct. 1). Results of uranyl phase analyses. Presented at the Seventh International Conference on the Chemistry and Migration Behavior of Actinides and Fission Products in the Geosphere. Lake Tahoe, CA.

*Publication Type: Proceeding*

Chen, F. & Ewing, R. C. (1999). 79-Se: Geochemical and crystallochemical retardation mechanisms. Symposium Proceedings of the Materials Research Society. 556, 1115-1122.



SEM-image of johanneite with precipitates of acicular gypsum on a sandstone sample from the Oklo open pit. [see Project #73751, renewal of 59849]

Chen, F. & Ewing, R. C. (1999). Structural contributions to the third-law entropy of uranyl phases. Symposium Proceedings of the Materials Research Society. 556, 1017-1024.

Ewing, R. C. (1999). Nuclear waste forms for actinides. Proceedings of the National Academy of Sciences. 96(7), 3432-3439.

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## **Separations Chemistry**

### **Project: 60392**

*Title:* Radiolytic and Thermal Process Relevant to Dry Storage of Spent Nuclear Fuels

*PI:* Dr. Steven C. Marschman

*Institution:* Pacific Northwest National Laboratory

*Publication Type:* Journal

Petrik, N. G., Alexandrov, A. B., Vall, A., & Orlando, T. M. (1999, in press). Gamma radiolysis of water on oxide surfaces: Parameters controlling the energy transfer.

Petrik, N. G., Taylor, D. P., & Orlando, T. M. (1999). Laser-stimulated luminescence of yttria-stabilized cubic-zirconia crystals. *J. Appl. Phys.* 85, 6770.

Simpson, W. C., Wang, W. K., Yarmoff, J. A., & Orlando, T. M. (1999). Photon- and electron-stimulated desorption of O<sup>+</sup> from zirconia. *Surf. Sci.* 423, 225.

*Publication Type:* Presentation

Haustein, P. (1999, Aug. 22-26). Nuclear stimulated desorption at the surfaces of model SNF materials: Experiment and computer simulation. Invited presentation at the Annual Symposium on First Accomplishments of the Environmental Management Science Program, American Chemical Society. New Orleans, LA.

Hedhili, M. N., Yakshinskiy, B. V., & Madey, T. E. (1999, Mar. 21-25). Interaction of water with UO<sub>2</sub> (001). National American Physical Society Meeting. Atlanta, GA.

Hedhili, M. N., Yakshinskiy, B. V., Madey, T. E., Dobrozemsky, R., & Yarmoff, J. (1999, Aug. 22-26). Interaction of water with uranium oxide surfaces. Annual Symposium on First Accomplishments of the Environmental Management Science Program. American Chemical Society. New Orleans, LA.

Orlando, T. M. (1999, Mar. 21-25). Quantum-resolved studies of condensed phase reactions. Invited presentation at the Annual Meeting of the Symposium on Free radicals in the Condensed Phase. American Chemical Society. Anaheim, CA.

Orlando, T. M., Petrik, N. G., Alexandrov, A. B., & Simpson, W. C. (1999, Feb. 26). Nonthermal processes on oxide surfaces and interfaces. Invited presentation at the Department of Chemistry, University of Utah. Salt Lake City, UT.

Orlando, T. M., Petrik, N. G., Alexandrov, A. B., & Simpson, W. C. (1999, Feb. 24-25). Nonthermal processes on oxide surfaces and interfaces. DOE Laboratory Catalysis Research Symposium. Albuquerque, NM.

Orlando, T. M., Petrik, N. G., Alexandrov, A. B., & Simpson, W. C. (1999, Feb. 24). Nonthermal processes on oxide surfaces and interfaces. Invited presentation at the Los Alamos National Laboratory. Los Alamos, NM.

Orlando, T. M., Petrik, N., Marshman, S., & Camaioni, D. M. (1999, Nov. 14-18). Nonthermal surface processes in the generation of gas in mixed wastes. Invited presentation at the Annual Meeting of the American Nuclear Society. Long Beach, CA.

Petrik, N., Marshman, S., Camaioni, D. M., & Orlando, T. M. (1999, Aug. 22-26). Nonthermal surface and interface processes in the storage of spent nuclear fuel and mixed wastes. Annual Symposium on First Accomplishments of the Environmental Management Science Program. American Chemical Society. New Orleans, LA.

## **SUBSURFACE CONTAMINATION**

### ***Actinide (Heavy Element) Chemistry***

**Project: 70050**

*Title:* Novel Optical Detection Schemes for In-Situ Mapping of Volatile Organochlorides in the Vadose Zone

*PI:* Dr. S. Michael Angel

*Institution:* University of South Carolina



Prototype coaxial fiber/electrode REMPI probe. [see Project #70050]

*Publication Type:* Poster

Chinni, R. C., et. al. (2000, Sept.). Resonance-enhanced multiphoton ionization (REMPI) measurements using visible excitation and a compact integrated fiber-optic probe. Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Nashville, TN.

*Publication Type:* Presentation

Angel, S. M., et. al. (2000, Nov. 28-30). In-situ resonance-enhanced multiphoton ionization (REMPI) measurements using a fiber-optic probe. FY2001 EMSP Vadose Zone Principal Investigator Workshop. Pacific Northwest National Laboratory. Richland, WA.